VARIATIONAL PRINCIPLE OF COUPLED HEAT AND MASS TRANSFER, TAKING THE FINITE PERTURBATION VELOCITY INTO ACCOUNT

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A variational principle for coupled heat and mass transfer is obtained for the case of finite perturbation velocity.

Both in describing heat conduction [1-4] and in studying phenomena of coupled heat and mass transfer [5-7], increasing attention has been paid recently to variational formulations of the problem and the development of variational methods of their solution. Most such works consider problems traditionally formulated using differential equation of parabolic type. However, it is known [8] that solutions obtained on the assumption of the infinite perturbation velocity in a number of cases give an idealized description of the transfer processes which contradicts the physical picture of the phenomenon.

The possibility of a variational approach to the investigation of coupled-transfer problems in the case when the transfer velocity is taken to be finite will now be demonstrated. First of all, the general case of a nonlinear problem is considered.

Suppose that inside an isotropic body of volume v, bounded by a surface S, there occurs a transfer process of n different substances under the action of n generalized forces. Let

$$h_k = \int_0^{\vartheta_k} c_k \gamma d\vartheta_k. \tag{1}$$

Here and below, the free index k is assumed to run over the values 1, 2,..., n. A dot above a symbol denotes the derivative with respect to time.

Consider the set of vector fields $\mathbf{H}_k = \mathbf{H}_k(x, y, z, t)$ satisfying the condition

$$\dot{\mathbf{H}}_k = \mathbf{j}_k, \tag{2}$$

where $\mathbf{j}_k$ is the specific flux of substances of type k.

The coupling of the flux densities of substances with the transfer potential gradients (the pulse velocity is finite) is written in the form

$$\mathbf{j}_k + t_{rk}\frac{\partial \mathbf{j}_k}{\partial t} = -\sum_{i=1}^{n} L_{ki}\,\mathrm{grad}\,\vartheta_i, \tag{3}$$

where $L_{ki} = L_{ki}(\vartheta)$ (i = 1, 2,..., n) are transfer coefficients.

Using Eq. (2), Eq. (3) may be rewritten in the form

$$\dot{\mathbf{H}}_k + t_{rk}\ddot{\mathbf{H}} = -\sum_{i=1}^{n} L_{ki}\,\mathrm{grad}\,\vartheta_i. \tag{4}$$

The conservation law for substances of type k in this case is written in the form

$$h_k = -\mathrm{div}\,\mathbf{H}_k \tag{5}$$

or for the variations δh_k and $\delta \mathbf{H}_k$ as

$$\delta h_k = -\mathrm{div}\,(\delta \mathbf{H}_k). \tag{6}$$

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The variational principle corresponding to the nonlinear problem is obtained by multiplying Eq. (4) by δH_k, integrating over the volume v with the use of the Ostrogradskii formula, and performing summation over k. Using Eq. (6), the result is

$$\int_v \sum_{k,i=1}^{n} \vartheta_i (L_{ki}\delta h_k - \operatorname{grad} L_{ki}\delta \mathbf{H}_k)\, dv + \int_v \sum_{k=1}^{n} (\dot{\mathbf{H}}_k + t_{rk}\ddot{\mathbf{H}}_k)\, \delta \mathbf{H}_k dv = -\int_S \sum_{k,i=1}^{n} \mathbf{n}\delta \mathbf{H}_k L_{ki}\vartheta_i dS, \tag{7}$$

where n is the unit vector of the external normal to the surface S.

The variational Eq. (7) is now formulated using the generalized Lagrangian coordinates $q_j = q_j(t)$ $(j = 1, 2, \ldots, m)$. Let

$$\mathbf{H}_k = \mathbf{H}_k(q_j, x, y, z, t), \quad \vartheta_k = \vartheta_k(q_j, x, y, z, t).$$

Then

$$\delta \mathbf{H}_k = \sum_{j=1}^{m} \frac{\partial \mathbf{H}_k}{\partial q_j}\delta q_j, \quad \delta h_k = \sum_{j=1}^{m} \frac{\partial h_k}{\partial q_j}\delta q_j\,. \tag{8}$$

Substituting Eq. (8) into Eq. (7), and taking the independence of variations of the generalized coordinates δq_j into account, it is found that

$$\int_v \sum_{k,i=1}^{n} \vartheta_i \left(L_{ki}\frac{\partial h_k}{\partial q_j} - \operatorname{grad} L_{ki}\frac{\partial \mathbf{H}_k}{\partial q_j}\right) dv + \int_v \sum_{k=1}^{n} (\dot{\mathbf{H}}_k + t_{rk}\ddot{\mathbf{H}}_k)\frac{\partial \mathbf{H}_k}{\partial q_j}\, dv = -\int_S \sum_{k,i=1}^{n} \mathbf{n}\frac{\partial \mathbf{H}_k}{\partial q_j} L_{ki}\vartheta_i dS \quad (j = 1, 2, \ldots, m). \tag{9}$$

Differentiating the vectors H_k with respect to time and the generalized coordinates, the following relations may be shown to hold

$$\frac{\partial \dot{\mathbf{H}}_k}{\partial \dot{q}_j} = \frac{\partial \mathbf{H}_k}{\partial q_j}, \quad \frac{\partial \ddot{\mathbf{H}}_k}{\partial \ddot{q}_j} = \frac{\partial \mathbf{H}_k}{\partial q_j}\,.$$

Then Eq. (9) takes the form

$$\frac{\partial D_1}{\partial \dot{q}_j} + \frac{\partial D_2}{\partial \ddot{q}_j} = V_j + Q_j \quad (j = 1, 2, \ldots, m), \tag{10}$$

where

$$D_1 = \frac{1}{2}\int_v \sum_{k=1}^{n} \dot{\mathbf{H}}_k^2\, dv; \quad D_2 = \frac{1}{2}\int_v \sum_{k=1}^{n} t_{rk}\ddot{\mathbf{H}}_k^2\, dv;$$

$$V_j = \int_v \sum_{k,i=1}^{n} \vartheta_i \left(\operatorname{grad} L_{ki}\frac{\partial \mathbf{H}_k}{\partial q_j} - L_{ki}\frac{\partial h_k}{\partial q_j}\right) dv;$$

$$Q_j = -\int_S \sum_{k,i=1}^{n} \mathbf{n}\frac{\partial \mathbf{H}_k}{\partial q_j} L_{ki}\vartheta_i dS.$$

The relation between the potentials ϑ_k and the vectors H_k in Eq. (10) are defined by Eq. (5).

Using generalized coordinates and Eq. (10), it is possible to introduce, for the approximate calculation of the transfer potential fields (taking the finite transfer velocity into account), the methods of reducing to ordinary differential equations, analogous to those used in [6, 7].

On the basis of the approach developed here, a variational principle is now constructed for the specific case of nonlinear coupled heat and mass transfer (n = 2) in the case when $\varepsilon\rho = \text{const}$. In this case [9]: ϑ_1 and ϑ_2 are heat and mass transfer potentials of the bound material; $\vartheta = (\vartheta_1, \vartheta_2)$; H_1 and H_2 are vector fields characterizing the heat and mass transfer, respectively; t_{r1} and t_{r2} are the relaxation times for heat and mass transfer, respectively; and

$$c_1 = c_q(\vartheta); \quad c_2 = c_m(\vartheta); \quad L_{11} = \lambda_q(\vartheta) + \varepsilon\rho\lambda_m(\vartheta)\,\delta(\vartheta), \quad L_{12} = \varepsilon\rho\lambda_m(\vartheta);$$
$$L_{21} = \lambda_m(\vartheta)\,\delta(\vartheta); \quad L_{22} = \lambda_m(\vartheta).$$

The variational principle in Eq. (7) now takes the form

$$\int_v \{[\vartheta_1(\lambda_q+\varepsilon\rho\lambda_m\delta)+\vartheta_2\varepsilon\rho\lambda_m]\,\delta h_1-[\vartheta_1 \operatorname{grad}(\lambda_q+\varepsilon\rho\lambda_m\delta)+$$
$$+\vartheta_2 \operatorname{grad}(\varepsilon\rho\lambda_m)]\,\delta\mathbf{H}_1+(\vartheta_1\lambda_m\delta+\vartheta_2\lambda_m)\,\delta h_2-[\vartheta_1 \operatorname{grad}(\lambda_m\delta)+$$
$$+\vartheta_2 \operatorname{grad}\lambda_m]\,\delta\mathbf{H}_2\}\,dv+\int_v [(\dot{\mathbf{H}}_1+t_{r1}\ddot{\mathbf{H}}_1)\,\delta\mathbf{H}_1+(\dot{\mathbf{H}}_2+t_{r2}\ddot{\mathbf{H}}_2)\,\delta\mathbf{H}_2]\,dv=$$
$$=-\int_S \{[\vartheta_1(\lambda_q+\varepsilon\rho\lambda_m\delta)+\vartheta_2\varepsilon\rho\lambda_m]\,\mathbf{n}\delta\mathbf{H}_1+(\vartheta_1\lambda_m\delta+\vartheta_2\lambda_m)\,\mathbf{n}\delta\mathbf{H}_2\}\,dS, \tag{11}$$

and Eq. (10) is written as

$$\frac{\partial D_1'}{\partial \dot{q}_j}+\frac{\partial D_2'}{\partial \ddot{q}_j}=-\int_v \{[\vartheta_1(\lambda_q+\varepsilon\rho\lambda_m\delta)+\vartheta_2\varepsilon\rho\lambda_m]\,\frac{\partial h_1}{\partial q_j}-$$
$$-[\vartheta_1 \operatorname{grad}(\lambda_q+\varepsilon\rho\lambda_m\delta)+\vartheta_2 \operatorname{grad}(\varepsilon\rho\lambda_m)]\,\frac{\partial \mathbf{H}_1}{\partial q_j}+(\vartheta_1\lambda_m\delta+\vartheta_2\lambda_m)\,\frac{\partial h_2}{\partial q_j}-$$
$$-[\vartheta_1 \operatorname{grad}(\lambda_m\delta)+\vartheta_2 \operatorname{grad}\lambda_m]\,\frac{\partial \mathbf{H}_2}{\partial q_j}\Big\}\,dv-\int_S \mathbf{n}\left\{\frac{\partial \mathbf{H}_1}{\partial q_j}\,[\vartheta_1(\lambda_q+\varepsilon\rho\lambda_m\delta)+\right.$$
$$\left.+\vartheta_2\varepsilon\rho\lambda_m]+\frac{\partial \mathbf{H}_2}{\partial q_j}\,(\vartheta_1\lambda_m\delta+\vartheta_2\lambda_m)\right\}dS \quad (j=1,\ 2,\ \ldots,\ m), \tag{12}$$

where

$$D_1'=\frac{1}{2}\int_v (\dot{\mathbf{H}}_1^2+\dot{\mathbf{H}}_2^2)\,dv;$$

$$D_2'=\frac{1}{2}\int_S (t_{r1}\ddot{\mathbf{H}}_1^2+t_{r2}\ddot{\mathbf{H}}_2^2)\,dv.$$

Setting $\lambda_m \equiv 0$ in Eqs. (11) and (12) leads to the heat-conduction problem ($\mathbf{H}_2 \equiv 0$) corresponding to finite heat-pulse velocity, when this process is described by the nonlinear differential equation [8]

$$\gamma(\vartheta)\,c(\vartheta)\left(\frac{\partial\vartheta}{\partial t}+t_r\,\frac{\partial^2\vartheta}{\partial t^2}\right)=\operatorname{div}(\lambda(\vartheta)\operatorname{grad}\vartheta). \tag{13}$$

In this case, Eqs. (11) and (12) give rise to a variational principle corresponding to Eq. (13) (the subscripts have been dropped)

$$\int_v \vartheta\delta h dv+\int_v \frac{1}{\lambda}\,(\dot{\mathbf{H}}+t_r\ddot{\mathbf{H}})\,\delta\mathbf{H}dv=-\int_S \vartheta\mathbf{n}\delta\mathbf{H}dS \tag{14}$$

and a system of equations in terms of the Lagrangian coordinates

$$\frac{\partial V}{\partial q_j}+\frac{\partial D_1''}{\partial \dot{q}_j}+\frac{\partial D_2''}{\partial \ddot{q}_j}=Q_j \quad (j=1,\ 2,\ \ldots,\ m), \tag{15}$$

where

$$V=\int_v\int_0^h \vartheta dh dv;\quad D_1''=\frac{1}{2}\int_v \frac{1}{\lambda}\,\dot{\mathbf{H}}^2 dv;$$

$$D_2''=\frac{t_r}{2}\int_v \frac{1}{\lambda}\,\ddot{\mathbf{H}}^2 dv;\quad Q_j=-\int_S \vartheta\mathbf{n}\,\frac{\partial \mathbf{H}}{\partial q_j}\,dS.$$

When $\gamma c=\text{const}$ and $\lambda=\text{const}$, Eq. (14) yields

$$\gamma c\int_v \vartheta\delta\vartheta dv+\frac{1}{\lambda}\int_v (\dot{\mathbf{H}}+t_r\ddot{\mathbf{H}})\,\delta\mathbf{H}dv=-\int_S \vartheta\mathbf{n}\delta\mathbf{H}dS.$$

This expression completely agrees with the variational principle obtained by Samoilovich [10] for the case when heat conduction is described by a linear equation of hyperbolic type, and after certain transformations Eq. (13) leads to the generalized Lagrange equations obtained in [10].

When $t_r \to 0$, Eqs. (14) and (15) lead to the variational principle of [2] for nonlinear heat conduction

$$\int_v \vartheta \delta h dv + \int_v \frac{1}{\lambda} \dot{\mathbf{H}} \delta \mathbf{H} dv = - \int_S \vartheta \mathbf{n} \delta \mathbf{H} dS$$

and the corresponding system of Lagrange equations.

The approach here proposed may also be used in investigating other problems leading to equations of hyperbolic type.

NOTATION

x, y, z, spatial coordinates; t, time; $\vartheta_k = \vartheta_k(x, y, z, t)$, excess (with respect to equilibrium) transfer potentials; $\vartheta = (\vartheta_1, \vartheta_2, \ldots, \vartheta_n)$; t_{rk}, relaxation time for a substance of type k; $c_k(\vartheta)$, specific heat for a substance of type k; $\gamma(\vartheta)$, density of body; c_q and c_m, specific heat and specific mass; λ_q and λ_m, thermal conductivity and mass conductivity; δ, Soret coefficient; ε and ρ, phase-conversion criterion and specific heat.

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